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13. ABSTRACT (Maximum 200 words) The main objective of this study is to develop an efficient multiscale coarse grid method which can be used as a competitive algorithm in studying composite materials and flow transport in strongly heterogeneous porous media. On one hand, we have explored the possibility of using adaptive mesh to reduce the modeling error introduced by the traditional moment average technique. On the other hand, we found that in the case of high aspect ratio permeability tensor, the modeling error in ignoring high order moments (3rd order or higher) could be very large. To overcome this difficulty, we have investigated an alternative approach that uses two-scale homogenization analysis to derive a coarse grid model in a systematic way. Finally, we have made some progress in developing numerical methods to solve multiscale nonlinear stochastic partial differential equations by using Wiener-Chaos expansions. These methods will reduce the problem of solving stochastic PDEs to solving a set of deterministic PDEs. This numerical method can be combined with our multiscale computational method, and can be used to compute accurately high order statistical quantities more efficiently than the traditional Monte-Carlo method.			
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Final Report for ARO Grant DAAD19-99-1-0141

PI: Thomas Y. Hou

Title of the proposal: Multi-Scale Finite Element Approximation for Transport in Heterogeneous Porous Media.

Funding Number: DAAD19-99-1-0141

Abstract.

The main objective of this study is to develop an efficient multiscale coarse grid method which can be used as a competitive algorithm in studying composite materials and flow transport in strongly heterogeneous porous media. On one hand, we have explored the possibility of using adaptive mesh to reduce the modeling error introduced by the traditional moment average technique. On the other hand, we found that in the case of high aspect ratio permeability tensor, the modeling error in ignoring high order moments (3rd order or higher) could be very large. To overcome this difficulty, we have investigated an alternative approach that uses two-scale homogenization analysis to derive a coarse grid model in a systematic way. Finally, we have made some progress in developing numerical methods to solve multiscale nonlinear stochastic partial differential equations by using Wiener-Chaos expansions. These methods will reduce the problem of solving stochastic PDEs to solving a set of deterministic PDEs. This numerical method can be combined with our multiscale computational method, and can be used to compute accurately high order statistical quantities more efficiently than the traditional Monte-Carlo method.

The Report Documentation Page:

I. Technical Accomplishments.

(1) The over-sampling technique and its error analysis.

One of the main difficulties in developing the multiscale computational methods is how to effectively localize the equation governing the small scales. If we use artificial boundary conditions from the large scales, such as linear boundary conditions, it will create mismatch among the small scales across the boundaries of coarse grid elements. Our analysis [6, 7] indicates that the error appears as a *resonance* between the small physical scales of the medium and the mesh size. Indeed the error is given by the ratio between the two scales; it increases as the size of grid blocks gets close to the small physical scales. We also show that the effect of different boundary conditions lies in a narrow region near the boundaries of grid blocks and it contributes to part of the resonance error. In [6], we introduced an *over-sampling* technique to remove the boundary layer effect. This is a very effective method that can be implemented easily for problems with many or continuous scales. This idea has recently been modified for the finite volume method and used in the new flow simulator code of Chevron.

A consequence of the over-sampling method is that the resulting multiscale finite element method is no longer conforming. With Efendiev and Wu [5], we give a detailed analysis of the non-conforming error. Our analysis also reveals a new cell resonance error which is caused by the mismatch between the mesh size and the wavelength of the small scale. We show that the cell resonance error is of lower order and is difficult to observe in practice.

(2). A mixed multiscale finite element method.

Recently, in collaboration with Dr. Z. Chen [4], we have developed a mixed multiscale finite element method. The advantage of a mixed finite element formulation is that the velocity flux is locally conserved across element boundaries. This is a very important property in many flow

simulations for large times. The violation of this local conservation property will lead to leakage of velocity flux. This will deteriorate the accuracy of the numerical solution for long time computations. This is the reason why mixed finite element methods are attractive for porous medium simulations. Our computational results have demonstrated convincingly that the mixed multiscale finite element method gives more accurate results for long time computations than the displacement multiscale finite element method.

(3). A PDE-based adaptive mesh generator.

In collaboration with Dr. Cenicerros [3], we have developed a new approach to generate a dynamically adaptive mesh for flows with singular layered structures. The use of well-resolved uniform meshes for this type of flows becomes prohibitively expensive. How to construct an effective moving meshes that can follow these singular layered structures *dynamically* is a very challenging problem. By solving a set of *nonlinear* elliptic equations, the mesh map is generated in a single step. The resulting adaptive method has the following attractive properties: (1) It is fast, with an optimal operation count $O(N)$, N is the number of grid points; (2) It can capture the *dynamical* evolution of singular structures without introducing artificial numerical diffusion; (3) It is highly accurate and stable. (4) It can be coupled easily with any existing PDE solver. We apply this dynamical moving mesh technique to study the evolution of an unstably stratified flow with three constant regions of densities connected by two thin layers. This is an extremely challenging problem. The flow develops very complex structure dynamically due to the Rayleigh-Taylor instability. The mesh effectively follows the flow throughout its complex evolution. The method is very stable and efficient during the entire computation.

(4). Combining multiscale modeling with mesh adaptivity

We have investigated the possibility of combining the multiscale finite element method with our PDE-based adaptive mesh generator. The adaptive mesh will be used to capture the dominant flow features, and the multiscale method will be used to capture the small scale effect within each coarse grid element by using moment average techniques. This will provide an effective coarse grid method for two-phase flows in heterogeneous media. My Ph.D. student, Andy Westhead, is now working at Exxon-Mobil as an intern for the second time to test this idea for realistic flow simulations. We are hopeful that this will lead to an improved accuracy in the upscaling model.

(5). Two-scale analysis for incompressible flows

A very common phenomenon in mechanics, physics, chemistry and engineering is that processes contain a wide range of spatial and temporal scales, which lead to rapidly varying structure in space and time. These include phase transitions, porous media flows, composite materials, acoustic waves and turbulent. The analysis of flows with rapidly varying structure is a very complex mathematical problem. Direct numerical simulations of these problems require tremendous amount of computer memory and CPU time which can easily exceed the limits of modern computing resources. Therefore, it is desirable to develop numerical methods which capture the effect of small scales on large scales using a relatively coarse grid.

Multiscale analysis for periodic structures (homogenization) has emerged as one of the successful techniques for these difficult problems with rapidly varying structure. The simplest multiscale analysis involves two scales. The first scale describes macroscopic quantities or slow variables. The second scale describes microscopic quantities or fast variables. Homogenization theory studies the relation between microscopic and macroscopic scales and provides effective equations for macroscopic quantities. It has been very successful in solving elliptic and parabolic problems with rapidly oscillating coefficients. But there has been only limited success in applying homogenization theory to hyperbolic problems.

Analysis of propagation of oscillations in incompressible Euler and Navier-Stokes equations has proved to be an extremely challenging problem. The pioneering work in this area was done by McLaughlin, Papanicolaou and Pironneau in their 1985 paper [12]. By using multiple scale analysis, they tried to obtain the homogenized equation for the incompressible Euler equation under the assumption that the highly oscillating part of the velocity field is transported only by the mean flow. This crucial assumption simplifies their multiscale analysis. However, this assumption is not very physical. In fact, there is no uniqueness of the cell problem they formulated. The existence of the cell problem is also open. Although a number of researchers have tried to resolve this difficulty, it is still one of the outstanding open questions in applied mathematics.

Recently, we have made some progress in deriving a homogenized equation for incompressible Euler equations in two and three space dimensions. The key idea is to perform multiscale expansions in the Lagrangian variable. The incompressible Euler equation is reduced to a nonlinear coupled system of the transport equation, which characterizes the flow map, and the elliptic problem for the stream function. Our multiscale analysis is carried out using this framework. This nonlinear coupled system describes the relation between large scales and small scales. It provides a beautiful mathematical model to understand complicated phenomenon of flows.

Our homogenization theory for the incompressible Euler equation with multi-scale initial data shows that the effect of small scale has only a local domain of influence. This enables us to develop an effective multiscale numerical method based on our asymptotic analysis which captures the correct large scale solution without making closure assumption. We plan to generalize our results to more general multiscale initial data without restrictive assumption on periodic structure and scale separation. We will also perform a number of numerical experiments to compare our results with the well-resolved solution and with other existing methods. Ultimately, we want to demonstrate that this two-scale analysis can be used to capture the large time behavior of the macroscopic solution for incompressible Navier-Stokes equations. If true, this will provide an effective numerical method for computing multiscale solution of incompressible flows.

(6). Numerical methods for solving stochastic PDEs

In practice, there are many physical processes that are governed by stochastic PDEs. Examples include wave propagation and diffusion through heterogeneous random media and the randomly forced Navier-Stokes equations. One commonly used method is the Monte Carlo method in which we simulate the problem realization by realization, and then average the solutions over many realizations. In each realization, one has to use a fine mesh to resolve the smallest scales introduced by the random perturbation. And one needs to perform many realizations in order to obtain accurate approximations to various statistical properties. The number of realizations could range from a few thousands to a few hundred thousands for problems with large variance.

Here we are interested in designing new type of numerical methods based on some well-known stochastic decompositions such as Karhunen-Loeve expansion [9], and Wiener-Chaos expansion [2]. Wiener-Chaos expansion represents any function $u(t, x, X_t)$ depending on a stochastic process X_t by

$$(1) \quad u(t, x, X_t) = \sum_n \frac{1}{\sqrt{n!}} \psi_n(t, x) \xi_n,$$

where ξ_n 's are Wick's polynomials (certain products of Hermite polynomials) which form a complete orthogonal basis of the probability functional space, and $\psi_n(t, x)$'s are their deterministic coefficients which are also computed by the inner product of u and ξ_n .

The most attractive point in Wiener-Chaos expansions is that the randomness of a stochastic process has been separated from its deterministic features. Therefore, we are able to derive equations for those deterministic coefficients and solve them using the standard methods. Once the

deterministic coefficients $\psi_n(t, x)$'s are available, it is easy to recover the statistics of the solutions from these coefficients. For example, the mean of the solutions is simple the first coefficient $\psi_0(t, x)$ in the expansion, and the variance is computed as:

$$(2) \quad E(v^2) = \sum_{\alpha} |v_{\alpha}|^2.$$

It has been proved [11] that finite sum approximations of Wiener-Chaos expansions is accurate with an error of the order $O(e^{ct}t^{N+1}/(N+1)!)$, where N is the number of terms in the Wiener-Chaos expansion. This suggests that if the Wiener-Chaos expansion is applied for a short time interval Δt , the approximation can achieve high accuracy. Based on this observation, we have designed a linear approximation scheme (with $N = 0$, which means only one linear term being used in the Wiener-Chaos expansion at every time interval with length Δt).

It has been verified numerically that when the variance of the force term is not large, especially when the fluctuation $\|(u')^2 - E((u')^2)\|$ is small, this linear scheme can give very accurate approximations to the statistical property. However, this linear scheme becomes insufficient when $\|(u')^2 - E((u')^2)\|$ is not small. In this case, it is necessary to include more terms (higher order Hermite polynomials) in the Wiener-Chaos expansion at every time interval to approximate the solution accurately. However, if we use the short time interval expansion as we did for the linear scheme, the number of Wiener-Chaos coefficients increases drastically since the nonlinearity of the equation brings all higher order coefficients, including the cross term coefficients between different time intervals. This could be computationally very expensive.

To alleviate this difficulty, we propose the following remedy. On one hand, we would like to limit the number of the Wiener-Chaos coefficients by using higher order Wiener-Chaos expansion. On the other hand, we would like to remain the accuracy and flexibility of short time interval approximations. To this end, we divide time interval $[0, t]$ into two subinterval $[0, t - \delta]$ and $[t - \delta, t]$, $\Delta t \ll \delta \ll 1$. The first subinterval corresponds to the earlier history of the Brownian motion which usually has small impact on the solution at the current time. The second subinterval corresponds to the short time contribution to the solution, which is not very smooth and requires high resolution. In both subintervals, we construct Wiener-Chaos expansions separately. Since there are only two subintervals, we can afford to compute the cross terms in the Wiener-Chaos expansions while retaining some higher order Wiener-Chaos expansions. Furthermore, the history term is relatively small and smooth. Only a small number of Wiener-Chaos coefficients are needed to obtain an accurate computation. Our preliminary results show that this strategy is both efficient and accurate.

(7). An Efficient Domain Decomposition Preconditioner for Multiscale Elliptic Problems with High Aspect Ratios

Many problems of fundamental and practical importance have multiple-scale solutions. Typical examples include transport of flows in strongly heterogeneous media and heat conduction in composite materials. When applying conventional FEM domain decomposition methods to these problems using linear or polynomial interpolations, the convergence rate deteriorates because the coarse grid solver does not account for fine scale heterogeneous features. To attain a satisfactory convergence rate it is therefore important to construct a coarse grid solver which reflects the small scale structures. Such a solver has been developed by Hou et al. [6, 7] who introduced the Multiscale Finite Element Method (MsFEM). The basic idea behind the MsFEM is to construct base functions which are adaptive to the local property of the differential operator and contain the important subgrid information.

An important property with the MsFEM solver is that the coarse approximation space is "generalized" discrete harmonic with respect to the physical elliptic operator that contains small scale coefficients. From a theoretical point of view, this property implies that the MsFEM solver is in

a sense optimal within a general class of coarse solvers. Furthermore it allows us to interpret the MsFEM solver as a natural extension of eg. linear finite elements to problems which include highly oscillatory coefficients. In particular, if the physical domain is partitioned into triangles or tetrahedrons and the elliptic coefficients are quasi-homogeneous, i.e. constant on each coarse grid element, then the corresponding MsFEM using linear boundary conditions to construct the multiscale base functions simply reduces to standard linear finite elements.

In [1] we develop, analyze and test a nonoverlapping domain decomposition preconditioner with the MsFEM solver as the coarse grid solver. The proposed preconditioner falls into the category of Schwarz methods, and the main steps in our analysis is based on the general abstract framework for the analysis of Schwarz methods. We first demonstrate that the MsFEM induces an ideal nonoverlapping domain decomposition preconditioner in 1D which converges in one iteration. In 2D and 3D the ability to select proper boundary conditions for the multiscale base functions will be important to achieve a fast convergence rate. In this paper, we only consider the case when the MsFEM solver is the "oscillatory extension" of linear finite elements. Our analysis shows that the proposed preconditioner gives the same rate of convergence for general elliptic problems with oscillatory coefficients as standard nonoverlapping domain decomposition methods using conventional coarse solvers achieve for elliptic problems with quasi-homogeneous coefficients. Moreover, we show that the condition number has only a relatively weak dependence on the local oscillatory coefficients and their aspect ratio.

We perform a series of numerical experiments to test the performance of our preconditioner for elliptic partial differential equations in two dimensions with highly oscillatory coefficients. We choose the coarse grid and the boundary conditions for the multiscale base functions so that the MsFEM solver is the "oscillatory extension" of bilinear finite elements. The elliptic coefficient function is chosen to be the product of a quasi-homogeneous coefficient function and a periodic oscillatory coefficient function. We demonstrate that the MsFEM induced preconditioner proposed in this paper shows a logarithmic dependence on the mesh ratio H/h and is almost insensitive to the local aspect ratios (for aspect ratios as high as 10^{10}). This confirms that the rate of convergence of our preconditioner for general elliptic problems with oscillatory coefficients is essentially the same as standard nonoverlapping domain decomposition methods using conventional coarse solvers achieve for elliptic problems with quasi-homogeneous coefficients. We compare our preconditioner with the preconditioners obtained by replacing the MsFEM solver with the linear and bilinear finite element solvers. The convergence behavior for these preconditioners deteriorates rapidly if the aspect ratio within the coarse grid elements blows up. As we are not aware of any other coarse solvers which successfully handles high aspect ratios, the linear and bilinear finite element solvers serve the purpose of illustrating the need for coarse solvers which can handle highly oscillatory coefficients.

(8). Singularity formation in 3D vortex sheets

One of the classical examples of hydrodynamic instability occurs when two fluids are separated by a free surface across which the tangential velocity has a jump discontinuity. This is called Kelvin-Helmholtz instability. Kelvin-Helmholtz instability is a fundamental instability of incompressible fluid flow at high Reynolds number. The idealization of a shear layered flow as a vortex sheet separating two regions of potential flow has often been used as a model to study mixing properties, boundary layers and coherent structures of fluids.

In collaboration with my former Ph.D. student, Gang Hu, [8], we have studied singularity formation of 3-D vortex sheets using a new approach. First, we derive a leading order approximation to the boundary integral equation governing the 3-D vortex sheet. This leading order equation captures the most singular contribution of the integral equation. Moreover, after applying a transformation to the physical variables, we found that this leading order 3-D vortex sheet equation de-generates

into a two-dimensional vortex sheet equation in the direction of the tangential velocity jump. This rather surprising result confirms that the tangential velocity jump is the physical driving force of the vortex sheet singularities. We show that the singularity type of the three-dimensional problem is similar to that of the two-dimensional problem.

In the March Issue of SIAM News (2002), there is a long feature article describing Yizhao's work with his Ph.D. student in studying singularity formation of three dimensional vortex sheets. The article concludes that "the new results of Hou and his colleagues have brought 'the ever distant goal' of understanding turbulence and hydrodynamic instability at least a few steps closer".

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II. List of manuscripts:

- [1] J. Aarnes and T. Y. Hou, *An Efficient Domain Decomposition Preconditioner for Multiscale Elliptic Problems with High Aspect Ratios*, Acta Mathematicae Applicatae Sinica 18 (1), 2002, pp. 63-76.
- [2] Z. M. Chen and T. Y. Hou, "A Mixed Finite Element Method for Elliptic Problems with Rapidly Oscillating Coefficients," to Math. Comput..
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- [5] T. Y. Hou and G. Hu, "Singularity Formation in 3-D Vortex Sheets," to appear in Phys. Fluids.
- [6] T. Y. Hou and G. Hu, "Long Time Existence of 3-D Vortex Sheets," to appear in Comm. PDEs.
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III. Scientific Personnel supported by this project.

Thomas Y. Hou (PI), Yalchin Efendiev (Ph.D. student), Andrew Westhead (Ph.D. student), Haomin Zhou (postdoc), Danping Yang (visiting associate).

VI. Technology Transfer:

The idea of the over-sampling method has been modified for the finite volume method and used in the new flow simulator code of Chevron. One of the unique features of the over-sampling method is to reduce the resonance error across coarse grid block boundary, and allows one to reconstruct the local fine grid velocity feature from the coarse grid calculation using the multiscale bases. My former Ph. D. student, Yalchin Efendiev, has contributed this technology transfer in a substantial way since he has been working very closely with the petroleum engineers there since he was a Ph.D. student at Caltech. Drs. Lou Durlofsky, Hamdi Tchelepi, and Seong Lee are our main contacts at Chevron Research Center.

V. Honors/awards/degrees received.

- (A). Thomas Y. Hou
 - (1) Recipient of 2001 James H. Wilkinson Prize in Numerical Analysis and Scientific Computing, SIAM, July, 2001.
 - (2) Invited Plenary Speaker, Invited Plenary Speaker, the Gordon Research Conference on Flow & Transport in Permeable Media, Andover, USA, August, 2002.
 - (3) Invited Plenary Speaker, the International Conference of Applied Mathematics in Memory of Jacques-Louis Lions, Paris, France, July 2002.

(4) Invited Plenary Speaker, the First SIAM/EMS Conference on Applied Mathematics in our Changing World, Berlin, Germany, September, 2001.

(5) Invited Plenary Speaker, Conference on Scientific Computing and Differential Equations, Scicade01, Vancouver, Canada, July, 2001.

(6) Invited Plenary Speaker, The Fourth European Conference on Numerical Mathematics and Advanced Applications, Ischia, Italy, July, 2001.

(7) Invited Plenary Speaker, the Third International Conference on Numerical Modeling in Continuum Mechanics, Prague, August, 2000.

(8) Invited Plenary Speaker, the Second International Conference on Boundary Integral Methods, Theory and Applications, Bath, UK, September, 2000.

(9) Invited Keynote Speaker, European Congress of Computational Methods in Applied Sciences and Engineering, Barcelona, Spain, September, 2000.

(10) Invited Plenary Speaker, the Thirteen International Conference on Domain Decomposition, Lyon, France, October, 2000.

(11) Invited Plenary Speaker, the Annual Meeting 2001 of the German Society for Applied Mathematics and Mechanics (GAMM), ETH Zurich, February, 2001.

(12) Invited Plenary Speaker, the International Conference on Scientific and Engineering Computing, Beijing, China, March, 2001.

(B). Degrees received

Yalchin Efendiev, a former Ph. D. student under the PI's supervision. He received his Ph.D. degree in Applied Math from Caltech in 1999.

Helen Si, a former Ph. D. student under the PI's supervision. She received his Ph.D. degree in Applied Math from Caltech in 2000.

Peter Park, a former Ph. D. student under the PI's supervision. She received his Ph.D. degree in Applied Math from Caltech in 2000.

Gang Hu, a former Ph. D. student under the PI's supervision. He received his Ph.D. degree in Applied Math from Caltech in 2001.

Dr. Efendiev received the 1999 Carey distinguished dissertation award in applied mathematics for his work on upscaling of flows through heterogeneous porous media.

Dr. Hu received the 2001 Carey distinguished dissertation award in applied mathematics for his work on singularity formation of three-dimensional vortex sheets.

VI. Others.

Founding a new SIAM journal on Multiscale Modeling and Simulation. Editor-in-Chief, 1/02 – present.